Simultaneous confidence intervals for the population cell means for 2×2 factorial data, utilizing prior information

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ABSTRACT

Consider a 2×2 factorial experiment with more than 1 replicate. Suppose that we have uncertain prior information that the two-factor interaction is zero. We describe new simultaneous frequentist confidence intervals for the 4 population cell means, with simultaneous confidence coefficient $1 - \alpha$, that utilize this prior information in the following sense. These simultaneous confidence intervals define a cube with expected volume that (a) is relatively small when the two-factor interaction is zero and (b) has maximum value that is not too large. Also, these intervals coincide with the standard simultaneous confidence intervals obtained by Tukey's method, with simultaneous confidence coefficient $1-\alpha$, when the data strongly contradict the prior information that the two-factor interaction is zero. We illustrate the application of these new simultaneous confidence intervals to a real data set.

Keywords: Prior information; simultaneous confidence intervals, 2-by-2 factorial data.

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1. Introduction

Consider a 2×2 factorial experiment with c replicates, where $c > 1$. Label the factors A and B. Suppose that the parameters of interest are the four population cell means $\theta_{00}, \theta_{10}, \theta_{01}, \theta_{11}$ where, for example, θ_{10} denotes the expected response when factor A is high and factor B is low. Also suppose that, on the basis of previous experience with similar data sets and/or expert opinion and scientific background, we have uncertain prior information that the two-factor interaction is zero. Our aim is to find simultaneous frequentist confidence intervals for the population cell means, with simultaneous confidence coefficient $1 - \alpha$, that utilize this prior information.

Similarly to Hodges and Lehmann [1], Bickel [2], Farchione and Kabaila [3], Kabaila and Giri [4,5] and Kabaila and Tuck [6], our aim is to utilize the uncertain prior information in the frequentist inference of interest, whilst providing a safeguard in case this prior information happens to be incorrect. Throughout this paper, we find that the simultaneous confidence intervals of interest define a cube. For convenience, we henceforth refer to this cube, rather than the corresponding simultaneous confidence intervals. Let $\theta = (\theta_{00}, \theta_{10}, \theta_{01}, \theta_{11})$. The standard $1 - \alpha$ confidence cube for θ is found using Tukey's method (described e.g. on p.289 of [7]). We assess a $1 - \alpha$ confidence cube for θ using the ratio (expected volume of this confidence cube)/(expected volume of standard $1 - \alpha$ confidence cube). We call this ratio the scaled expected volume of this confidence cube. We say that this confidence cube utilizes the prior information if it has the following desirable properties. This confidence cube has scaled expected volume that (a) is significantly less than 1 when the two-factor interaction is zero and (b) has a maximum value that is not too much larger than 1. Also, this confidence cube coincides with the standard $1 - \alpha$ confidence cube when the data strongly contradict the prior information that the two-factor interaction is zero.

An attempt to utilize the uncertain prior information is as follows. We carry out a preliminary test of the null hypothesis that the two-factor interaction is zero against the alternative hypothesis that it is non-zero. If this null hypothesis is accepted then the confidence cube for θ, with nominal confidence coefficient $1 - \alpha$, is constructed assuming that it is known *a priori* that the two-factor interaction is zero; otherwise

the standard $1-\alpha$ confidence cube is used. We call this the naive $1-\alpha$ confidence cube for θ. This assumption is false and it leads to a naive $1-\alpha$ confidence cube with minimum coverage probability less than $1-\alpha$. For example, for $\alpha = 0.05$, $c = 2$ and a preliminary test with level of significance 0.05, this minimum coverage probability is 0.9078. The poor coverage properties of these naive confidence cubes are presaged by the following two strands of literature. The first strand concerns the poor properties of inferences about main effects after preliminary hypothesis tests in factorial experiments, see e.g. Neyman [8], Traxler [9], Bohrer and Sheft [10], Fabian [11], Shaffer [12] and Ng [13]. The second strand concerns the poor coverage properties of naive (non-simultaneous) confidence intervals in the context of linear regression models with zero-mean normal errors, see e.g. Kabaila [14, 15], Kabaila and Leeb [16], Giri and Kabaila [17] and Kabaila and Giri [18].

Whilst the naive $1-\alpha$ confidence cube fails to properly utilize the prior information, its form (described in Section 2) will be used to provide some motivation for the new $1-\alpha$ confidence cube that utilizes the uncertain prior information and is described in Section 3. In this section we also provide a numerical illustration of the properties of this new confidence cube for $1-\alpha = 0.95$ and $c = 2$. The two-factor interaction is described by the parameter β_{12} in the regression model used for the experiment. The uncertain prior information is that $\beta_{12} = 0$. Define the parameter $\gamma = \beta_{12}/\sqrt{\text{var}(\hat{\beta}_{12})}$, where $\hat{\beta}_{12}$ denotes the least squares estimator of β_{12}. As proved in Section 3, the scaled expected volume of the new confidence cube for θ is an even function of γ. The bottom panel of Figure 2 is a plot of the square root of the scaled expected volume of the new 0.95 confidence cube for θ, as a function of γ. When the prior information is correct (i.e. $\gamma = 0$), we gain since the square root of the scaled expected volume is substantially smaller than 1. The maximum value of the square root of the scaled expected volume is not too large. The new 0.95 confidence interval for θ coincides with the standard $1-\alpha$ confidence cube when the data strongly contradicts the prior information. This is reflected in Figure 2 by the fact that the square root of the scaled expected volume approaches 1 as $\gamma \to \infty$. In Section 4 we illustrate the application of the new $1-\alpha$ confidence cube to a real data set.

2. The naive $1-\alpha$ confidence cube

Let Y denote the response and x_1 and x_2 denote the coded levels for factor A and factor B respectively, where x_1 takes values -1 and 1 when the factor A takes the values low and high respectively and x_2 takes values -1 and 1 when the factor B takes the values low and high respectively. We assume the model

$$Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \varepsilon \tag{1}$$

where β_0, β_1, β_2 and β_{12} are unknown parameters and the ε for different response measurements are independent and identically $N(0, \sigma^2)$ distributed. Because we are considering c replicates, the number of measurements of the response is $n = 4c$. The dimension of the regression parameter vector $(\beta_0, \beta_1, \beta_2, \beta_{12})$ is $p = 4$. The parameters of interest are $\theta_{00} = \beta_0 - \beta_1 - \beta_2 + \beta_{12}$, $\theta_{10} = \beta_0 + \beta_1 - \beta_2 - \beta_{12}$, $\theta_{01} = \beta_0 - \beta_1 + \beta_2 - \beta_{12}$ and $\theta_{11} = \beta_0 + \beta_1 + \beta_2 + \beta_{12}$. The uncertain prior information is that $\beta_{12} = 0$.

The naive $1-\alpha$ confidence cube is defined as follows. We carry out a preliminary test of the null hypothesis that $\beta_{12} = 0$ against the alternative hypothesis that $\beta_{12} \neq 0$. If this null hypothesis is accepted then the confidence cube is constructed assuming that it was known *a priori* that $\beta_{12} = 0$; otherwise the standard $1-\alpha$ confidence cube for θ is used.

Let $\big(\hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_{12}\big)$ denote the least squares estimator of $\big(\beta_0, \beta_1, \beta_2, \beta_{12}\big)$. Also, let $\big(\hat{\Theta}_{00}, \hat{\Theta}_{10}, \hat{\Theta}_{01}, \hat{\Theta}_{11}\big)$ denote the least squares estimator of $\big(\theta_{00}, \theta_{10}, \theta_{01}, \theta_{11}\big)$. Note that $\big(\hat{\Theta}_{00}, \hat{\Theta}_{10}, \hat{\Theta}_{01}, \hat{\Theta}_{11}, \hat{\beta}_{12}\big)$ has a multivariate normal distribution with mean $\big(\theta_{00}, \theta_{10}, \theta_{01}, \theta_{11}, \beta_{12}\big)$ and covariance matrix $\sigma^2 V$, where

$$V = \frac{1}{4c}\begin{bmatrix} 4 & 0 & 0 & 0 & 1 \\ 0 & 4 & 0 & 0 & -1 \\ 0 & 0 & 4 & 0 & -1 \\ 0 & 0 & 0 & 4 & 1 \\ 1 & -1 & -1 & 1 & 1 \end{bmatrix}$$

Let v_{ij} denote the (i, j) th element of V. Also, let $\hat{\sigma}^2$ denote the usual estimator of σ^2 obtained by fitting the the full model to the data. Define $W = \hat{\sigma}/\sigma$. Note that W has the same distribution as $\sqrt{Q/(n-p)}$ where $Q \sim \chi^2_{n-p}$. Let f_W denote the probability density function of W. Define $d_{1-\alpha}$ by $P\big(\max_{i=1,\ldots,4} |Z_i|/W \leq d_{1-\alpha}\big) =$

$1-\alpha$, where Z_1, Z_2, Z_3, Z_4 and W independent random variables and $Z_i \sim N(0,1)$ $(i=1,2,3,4)$. We use $[a \pm b]$ to denote the interval $[a-b, a+b]$. The standard $1-\alpha$ confidence cube for θ is

$$I = \left[\hat{\Theta}_{00} \pm d_{1-\alpha}\sqrt{v_{11}}\hat{\sigma}\right] \times \left[\hat{\Theta}_{10} \pm d_{1-\alpha}\sqrt{v_{22}}\hat{\sigma}\right] \\ \times \left[\hat{\Theta}_{01} \pm d_{1-\alpha}\sqrt{v_{33}}\hat{\sigma}\right] \times \left[\hat{\Theta}_{11} \pm d_{1-\alpha}\sqrt{v_{44}}\hat{\sigma}\right].$$

The naive $1-\alpha$ confidence cube for θ is obtained as follows. The usual test statistic for testing the null hypothesis that $\beta_{12}=0$ against the alternative hypothesis that $\beta_{12} \neq 0$ is $\hat{\beta}_{12}/(\hat{\sigma}\sqrt{v_{55}})$. This test statistic has a t_{n-p} distribution under this null hypothesis. Suppose that, for some given positive number q, we fix β_{12} at 0 if $|\hat{\beta}_{12}|/(\hat{\sigma}\sqrt{v_{55}}) \leq q$; otherwise we allow β_{12} to vary freely. Define $\tilde{\sigma}^2 = \big((n-p)\hat{\sigma}^2 + (\hat{\beta}_{12}^2/v_{55})\big)/(n-p+1)$. This is the usual estimator of σ^2 obtained by fitting the full model to the data when it is assumed that $\beta_{12}=0$. Define $\tilde{W} = \tilde{\sigma}/\sigma$. Note that $\tilde{W}$ has the same distribution as $\sqrt{\tilde{Q}/(n-p+1)}$, where $\tilde{Q} \sim \chi^2_{n-p+1}$ when $\beta_{12}=0$. Suppose that Z_1, Z_2, Z_3 and $\tilde{W}$ are independent random variables and $Z_i \sim N(0,1)$ $(i=1,2,3)$. Let $\tilde{Z}_1 = (Z_1 - Z_2 - Z_3)/\sqrt{3}$, $\tilde{Z}_2 = (Z_1 + Z_2 - Z_3)/\sqrt{3}$, $\tilde{Z}_3 = (Z_1 - Z_2 + Z_3)/\sqrt{3}$ and $\tilde{Z}_4 = (Z_1 + Z_2 + Z_3)/\sqrt{3}$. Define $\tilde{d}_{1-\alpha}$ by $P\big(\max_{i=1,\ldots,4}|\tilde{Z}_i|/\tilde{W} \leq \tilde{d}_{1-\alpha}\big) = 1-\alpha$. The naive $1-\alpha$ confidence cube is obtained as follows. If $|\hat{\beta}_{12}|/(\hat{\sigma}\sqrt{v_{55}}) > q$ then this confidence cube is I. If, on the other hand, $|\hat{\beta}_{12}|/(\hat{\sigma}\sqrt{v_{55}}) \leq q$ then this confidence cube is

$$\big[\hat{\Theta}_{00} - \hat{\beta}_{12} \pm (\sqrt{3/c}/2)\tilde{d}_{1-\alpha}\tilde{\sigma}\big] \times \big[\hat{\Theta}_{10} + \hat{\beta}_{12} \pm (\sqrt{3/c}/2)\tilde{d}_{1-\alpha}\tilde{\sigma}\big] \\ \times \big[\hat{\Theta}_{01} + \hat{\beta}_{12} \pm (\sqrt{3/c}/2)\tilde{d}_{1-\alpha}\tilde{\sigma}\big] \times \big[\hat{\Theta}_{110} - \hat{\beta}_{12} \pm (\sqrt{3/c}/2)\tilde{d}_{1-\alpha}\tilde{\sigma}\big]$$

The naive $1-\alpha$ confidence cube can be expressed in the form

$$\left[\hat{\Theta}_{00} - \sqrt{v_{11}}\hat{\sigma}\, b\left(\frac{\hat{\beta}_{12}}{\hat{\sigma}\sqrt{v_{55}}}\right) \pm \sqrt{v_{11}}\hat{\sigma}\, s\left(\frac{|\hat{\beta}_{12}|}{\hat{\sigma}\sqrt{v_{55}}}\right)\right] \\ \times \left[\hat{\Theta}_{10} + \sqrt{v_{22}}\hat{\sigma}\, b\left(\frac{\hat{\beta}_{12}}{\hat{\sigma}\sqrt{v_{55}}}\right) \pm \sqrt{v_{22}}\hat{\sigma}\, s\left(\frac{|\hat{\beta}_{12}|}{\hat{\sigma}\sqrt{v_{55}}}\right)\right] \\ \times \left[\hat{\Theta}_{01} + \sqrt{v_{33}}\hat{\sigma}\, b\left(\frac{\hat{\beta}_{12}}{\hat{\sigma}\sqrt{v_{55}}}\right) \pm \sqrt{v_{33}}\hat{\sigma}\, s\left(\frac{|\hat{\beta}_{12}|}{\hat{\sigma}\sqrt{v_{55}}}\right)\right] \\ \times \left[\hat{\Theta}_{11} - \sqrt{v_{44}}\hat{\sigma}\, b\left(\frac{\hat{\beta}_{12}}{\hat{\sigma}\sqrt{v_{55}}}\right) \pm \sqrt{v_{44}}\hat{\sigma}\, s\left(\frac{|\hat{\beta}_{12}|}{\hat{\sigma}\sqrt{v_{55}}}\right)\right] \qquad (2)$$

where

$$b(x) = \begin{cases} 0 & \text{for} \quad |x| > q \\ x/2 & \text{for} \quad |x| \le q. \end{cases}$$

$$s(x) = \begin{cases} d_{1-\alpha} & \text{for} \quad x > q \\ \tilde{d}_{1-\alpha}(\sqrt{3}/2)\sqrt{(n-p+x^2)/(n-p+1)} & \text{for} \quad 0 < x \le q. \end{cases}$$

3. New $1-\alpha$ confidence cube utilizing the prior information

We introduce a confidence cube for θ that is similar in form to the naive $1-\alpha$ confidence cube, described in the previous section, but with a great "loosening up" of the forms that the functions b and s can take. Define the confidence cube $J(b,s)$ for θ to have the form (2), where the functions b and s are required to satisfy the following restriction.

Restriction 1 $b : \mathbb{R} \to \mathbb{R}$ is an odd function and $s : [0,\infty) \to [0,\infty)$.

Invariance arguments, of the type used by Farchione and Kabaila [3] and Kabaila and Giri [4], may be used to motivate this restriction. For the sake of brevity, these arguments are omitted. We also require the functions b and s to satisfy the following restriction.

Restriction 2 b and s are continuous functions.

This implies that the endpoints of the simultaneous confidence intervals corresponding to the confidence cube $J(b,s)$ are continuous functions of the data. Finally, we require the confidence cube $J(b,s)$ to coincide with the standard $1-\alpha$ confidence cube I when the data strongly contradict the prior information. The statistic $|\hat{\beta}_{12}|/(\hat{\sigma}\sqrt{v_{22}})$ provides some indication of how far away $\beta_{12}/(\sigma\sqrt{v_{22}})$ is from 0. We therefore require that the functions b and s satisfy the following restriction.

Restriction 3 $b(x) = 0$ for all $|x| \ge r$ and $s(x) = d_{1-\alpha}$ for all $x \ge r$ where r is a (sufficiently large) specified positive number.

Define $\gamma = \beta_{12}/(\sigma\sqrt{v_{55}})$, $T_1 = (\hat{\beta}_0 - \beta_0)/(\sigma\sqrt{v_{55}})$, $T_2 = (\hat{\beta}_1 - \beta_1)/(\sigma\sqrt{v_{55}})$, $T_3 = (\hat{\beta}_2 - \beta_2)/(\sigma\sqrt{v_{55}})$ and $H = \hat{\beta}_{12}/(\sigma\sqrt{v_{55}})$. Then define $G_1 = (T_1 - T_2 - T_3 + H - \gamma)/2$, $G_2 = (T_1 + T_2 - T_3 - H + \gamma)/2$, $G_3 = (T_1 - T_2 + T_3 - H + \gamma)/2$, $G_4 = (T_1 + T_2 + T_3 + H - \gamma)/2$. Note that $H \sim N(\gamma, 1)$. It is straightforward to

show that the coverage probability $P\big(\theta \in J(b,s)\big)$ is equal to

$$P\big(\ell(H,W) \le G_1 \le u(H,W),\, \ell(H,W) \le -G_2 \le u(H,W),\\ \ell(H,W) \le -G_3 \le u(H,W),\, \ell(H,W) \le G_4 \le u(H,W)\big) \quad (3)$$

where the functions $\ell(\cdot,\cdot) : \mathbb{R} \times [0,\infty) \to \mathbb{R}$ and $u(\cdot,\cdot) : \mathbb{R} \times [0,\infty) \to \mathbb{R}$ are defined by $\ell(h,w) = b(h/w)w - s(|h|/w)w$ and $u(h,w) = b(h/w)w + s(|h|/w)w$. As we prove later, for given b and s, the coverage probability of $J(b,s)$ is an even function of γ. We denote this coverage probability by $c(\gamma; b, s)$.

Part of our evaluation of the confidence cube $J(b,s)$ consists of comparing it with the standard $1-\alpha$ confidence cube I using the criterion

$$\frac{\text{expected volume of } J(b,s)}{\text{expected volume of } I}.$$

We call this the scaled expected volume of $J(b,s)$. This is equal to

$$\frac{E\left(W^4\, s^4\left(\dfrac{|H|}{W}\right)\right)}{d_{1-\alpha}^4\, E(W^4)}.$$

This is a function of γ for given s. We denote this function by $e(\gamma; s)$. Clearly, for given function s, $e(\gamma; s)$ is an even function of γ. When $J(b,s)$ is a $1-\alpha$ confidence cube, we use $\sqrt{e(\gamma; s)}$ to measure the efficiency of the standard $1-\alpha$ confidence cube relative to $J(b,s)$, for parameter value γ. The reason for this is that $\sqrt{e(\gamma; s)}$ is a measure of the ratio of sample sizes required for the expected volumes of these two confidence cubes to be equal.

Our aim is to find functions b and s that satisfy Restrictions 1–3 and such that (a) the minimum of $c(\gamma; b, s)$ over γ is $1-\alpha$ and (b) the weighted average

$$\int_{-\infty}^{\infty} (e(\gamma; s) - 1)\, d\nu(\gamma) \quad (4)$$

is minimized, where the weight function ν has been chosen to be

$$\nu(x) = \lambda x + \mathcal{H}(x) \quad \text{for all} \quad x \in \mathbb{R}, \quad (5)$$

where λ is a specified nonnegative number and $\mathcal{H}$ is the unit step function defined by $\mathcal{H}(x) = 0$ for $x < 0$ and $\mathcal{H}(x) = 1$ for $x \ge 0$. The larger the value of λ, the smaller

the relative weight given to minimizing $e(\gamma; s)$ for $\gamma = 0$, as opposed to minimizing $e(\gamma; s)$ for other values of γ. The idea of minimizing a weighted average expected length of a confidence interval, subject to a coverage probability constraint, is due to Pratt [19]. The particular weight function (5) was first used in related contexts by Farchione and Kabaila [3] and Kabaila and Giri [4].

The following theorem provides computationally convenient expressions for the coverage probability and scaled expected length of $J(b, s)$.

Theorem 1.

(a) *Define* $\ell_1 = 2\ell(h, w) + t_3 - h + \gamma$, $u_1 = 2u(h, w) + t_3 - h + \gamma$, $\ell_2 = -2u(h, w) + t_3 + h - \gamma$ *and* $u_2 = -2\ell(h, w) + t_3 + h - \gamma$. *Now define* $\tilde{\ell}_1 = \max(\ell_1, -u_1)$, $\tilde{u}_1 = \min(u_1, -\ell_1)$, $\tilde{\ell}_2 = \max(\ell_2, -u_2)$ *and* $\tilde{u}_2 = \min(u_2, -\ell_2)$. *We use these functions to define*

$$k(t_3, h, w, \gamma) = \begin{cases} 0 \text{ if either } \tilde{\ell}_1 > \tilde{u}_1 \text{ or } \tilde{\ell}_2 > \tilde{u}_2, \\ \Big(\Phi\big(\tilde{u}_1/\sqrt{2}\big) - \Phi\big(\tilde{\ell}_1/\sqrt{2}\big)\Big)\Big(\Phi\big(\tilde{u}_2/\sqrt{2}\big) - \Phi\big(\tilde{\ell}_2/\sqrt{2}\big)\Big) \text{ otherwise,} \end{cases}$$

where Φ *denotes the* $N(0,1)$ *distribution function.*

Define $\ell^\dagger(w) = -d_{1-\alpha} w$ *and* $u^\dagger(w) = d_{1-\alpha} w$. *Also define* $\ell_1^\dagger = 2\ell^\dagger(w) + t_3 - h + \gamma$, $u_1^\dagger = 2u^\dagger(w) + t_3 - h + \gamma$, $\ell_2^\dagger = -2u^\dagger(w) + t_3 + h - \gamma$ *and* $u_2^\dagger = -2\ell^\dagger(w) + t_3 + h - \gamma$. *Now define* $\tilde{\ell}_1^\dagger = \max(\ell_1^\dagger, -u_1^\dagger)$, $\tilde{u}_1^\dagger = \min(u_1^\dagger, -\ell_1^\dagger)$, $\tilde{\ell}_2^\dagger = \max(\ell_2^\dagger, -u_2^\dagger)$ *and* $\tilde{u}_2^\dagger = \min(u_2^\dagger, -\ell_2^\dagger)$. *We use these functions to define*

$$k^\dagger(t_3, h, w, \gamma) = \begin{cases} 0 \text{ if either } \tilde{\ell}_1^\dagger > \tilde{u}_1^\dagger \text{ or } \tilde{\ell}_2^\dagger > \tilde{u}_2^\dagger, \\ \Big(\Phi\big(\tilde{u}_1^\dagger/\sqrt{2}\big) - \Phi\big(\tilde{\ell}_1^\dagger/\sqrt{2}\big)\Big)\Big(\Phi\big(\tilde{u}_2^\dagger/\sqrt{2}\big) - \Phi\big(\tilde{\ell}_2^\dagger/\sqrt{2}\big)\Big) \text{ otherwise.} \end{cases}$$

The coverage probability of $J(b, s)$, *denoted by* $c(\gamma; b, s)$, *is equal to*

$$(1-\alpha) + \int_0^\infty \int_{-r}^{r} \int_{-\infty}^{\infty} \big(k(t_3, wx, w, \gamma) - k^\dagger(t_3, wx, w, \gamma)\big)\, \phi(t_3)\, dt_3\, \phi(wx - \gamma)\, dx\, w\, f_W(w)\, dw \tag{6}$$

where ϕ *denotes the* $N(0,1)$ *probability density function. For given functions* b *and* s, $c(\gamma; b, s)$ *is an even function of* γ.

(b) *The scaled expected volume of* $J(b, s)$, *denoted by* $e(\gamma; s)$, *is equal to*

$$1 + \frac{1}{d_{1-\alpha}^4\, E(W^4)} \int_0^\infty \int_{-r}^{r} \big(s^4(|x|) - d_{1-\alpha}^4\big)\, \phi(wx - \gamma)\, dx\, w^5\, f_W(w)\, dw. \tag{7}$$

This theorem is proved in the Appendix. Substituting (7) into (4), we obtain that (4) is equal to

$$
\begin{aligned}
&\frac{1}{d_{1-\alpha}^4\, E(W^4)} \int_{-\infty}^{\infty} \int_0^{\infty} \int_{-r}^{r} \left(s^4(|x|) - d_{1-\alpha}^4\right) \phi(wx-\gamma)\, dx\, w^5\, f_W(w)\, dw\, d\nu(\gamma) \\
&= \frac{1}{d_{1-\alpha}^4\, E(W^4)} \int_0^{\infty} \int_{-r}^{r} \left(s^4(|x|) - d_{1-\alpha}^4\right) \int_{-\infty}^{\infty} \phi(wx-\gamma)\, d\nu(\gamma)\, dx\, w^5\, f_W(w)\, dw \\
&= \frac{2}{d_{1-\alpha}^4\, E(W^4)} \int_0^{\infty} \int_0^{r} \left(s^4(x) - d_{1-\alpha}^4\right) \left(\lambda + \phi(wx)\right) dx\, w^5\, f_W(w)\, dw \qquad (8)
\end{aligned}
$$

For computational feasibility, we specify the following parametric forms for the functions b and s. We require b to be a continuous function and so it is necessary that $b(0) = 0$. Suppose that $x_1, \ldots, x_m$ satisfy $0 = x_1 < x_2 < \cdots < x_m = r$. Obviously, $b(x_1) = 0$, $b(x_m) = 0$ and $s(x_m) = d_{1-\alpha}$. The function b is fully specified by the vector $\big(b(x_2), \ldots, b(x_{m-1})\big)$ as follows. Because b is assumed to be an odd function, we know that $b(-x_i) = -b(x_i)$ for $i = 2, \ldots, m$. We specify the value of $b(x)$ for any $x \in [-r, r]$ by cubic spline interpolation for these given function values, subject to the constraint that $b'(-r) = 0$ and $b'(r) = 0$. We fully specify the function s by the vector $\big(s(x_1), \ldots, s(x_{m-1})\big)$ as follows. The value of $s(x)$ for any $x \in [0, r]$ is specified by cubic spline interpolation for these given function values (without any endpoint conditions on the first derivative of s). We call $x_1, x_2, \ldots x_m$ the knots.

To conclude, the new $1-\alpha$ confidence cube for θ that utilizes the uncertain prior information that $\beta_{12} = 0$ is obtained as follows. For a judiciously-chosen set of values of r, λ and knots x_i, we carry out the following computational procedure.

Computational Procedure

Compute the functions b and s, satisfying Restrictions 1–3 and taking the parametric forms described above, such that (a) the minimum over $\gamma \geq 0$ of (6) is $1-\alpha$ and (b) the criterion (8) is minimized. Plot $\sqrt{e(\gamma; s)}$ as a function of $\gamma \geq 0$.

Based on these plots and the strength of our prior information that $\beta_{12} = 0$, we choose appropriate values of r, λ and knots x_i. The confidence cube corresponding to this choice is the new $1-\alpha$ confidence cube for θ.

Consider the case that $c = 2$ and $1-\alpha = 0.95$. We followed this Computational Procedure, with $r = 8$, $\lambda = 0.08$ and evenly-spaced knots x_i at $0, r/6, \ldots, r$. The resulting functions b and s, which specify the new 0.95 confidence cube for θ are plotted in Figure 1. The performance of this confidence cube is shown in Figure

2. This confidence cube has the attractive property that its coverage probability is 0.95 throughout the parameter space. When the prior information is correct (i.e. $\gamma = 0$), we gain since $\sqrt{e(0; s)} = 0.8558$. The maximum value of $\sqrt{e(\gamma; s)}$ is 1.0956. This confidence cube coincides with the standard 0.95 confidence cube for θ when the data strongly contradicts the prior information, so that $\sqrt{e(\gamma; s)}$ approaches 1 as $\gamma \to \infty$.

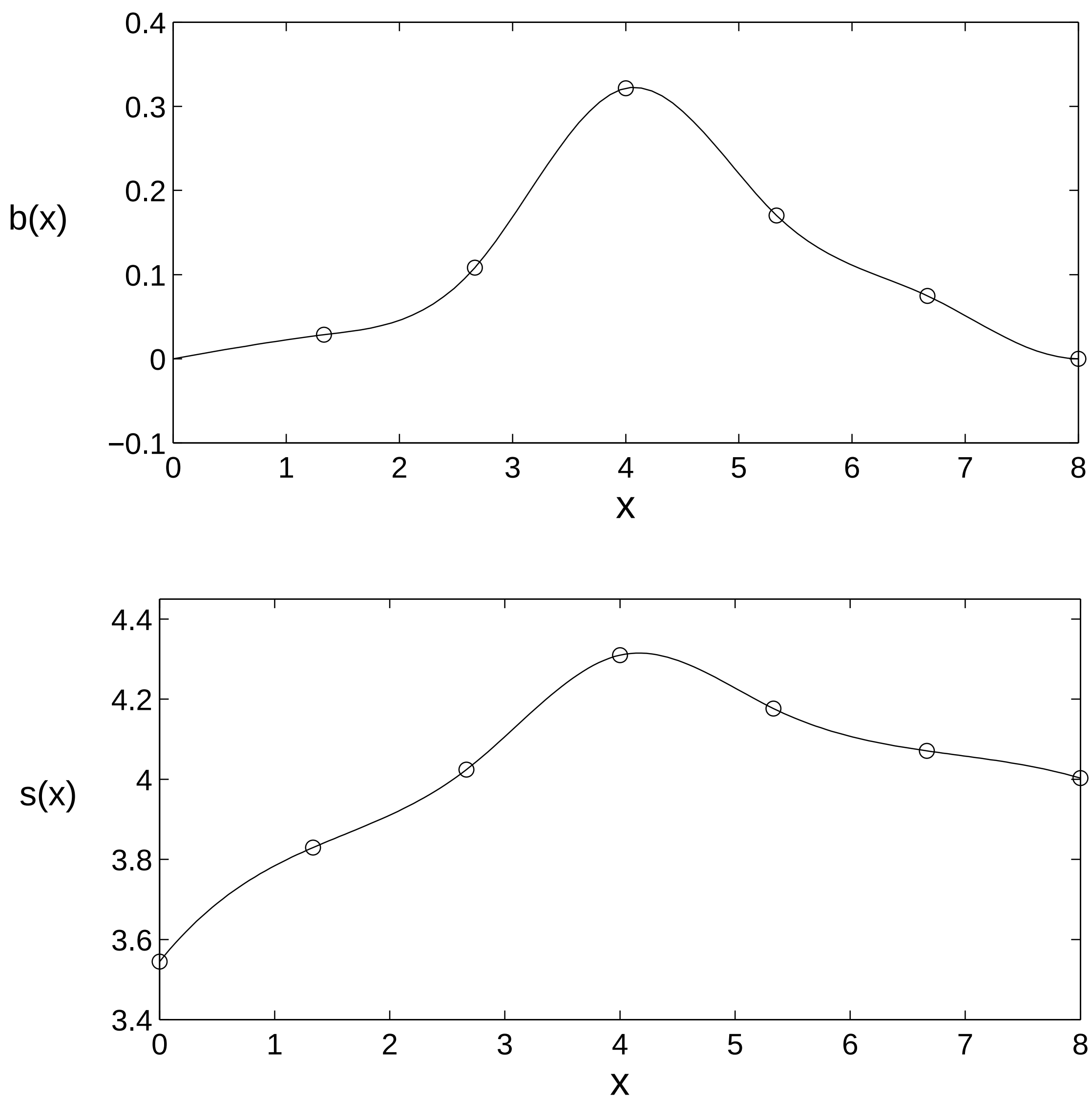

Figure 1: Plots of the functions b and s that specify the new 0.95 confidence cube for $\theta = (\theta_{00}, \theta_{10}, \theta_{01}, \theta_{12})$, when $c = 2$, $r = 8$ and $\lambda = 0.08$.

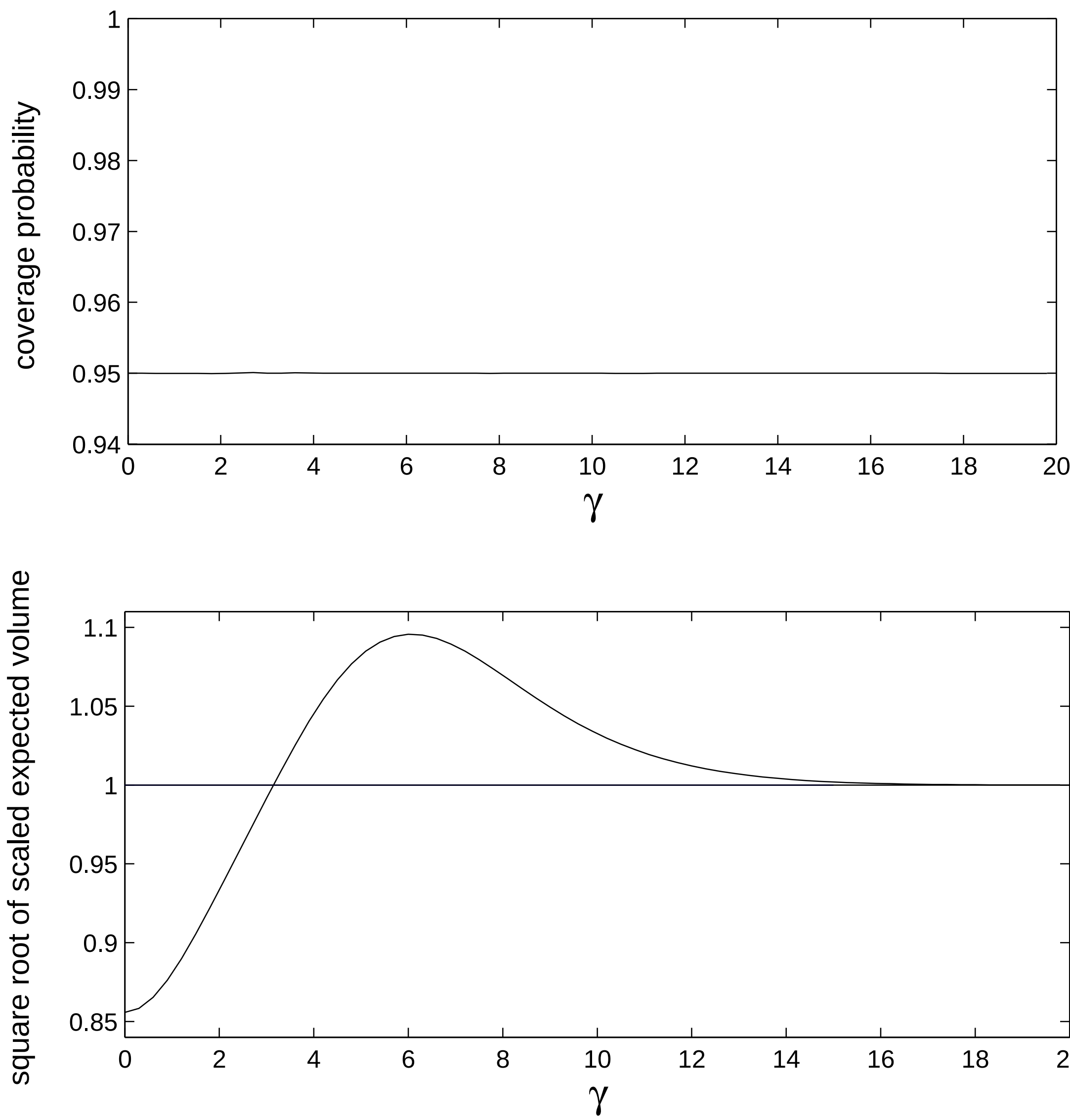

Figure 2: Plots of the coverage probability and the square root of the scaled expected volume $e(\gamma; s)$ $\big($as functions of $\gamma = \beta_{12}/\sqrt{\mathrm{var}(\hat{\beta}_{12})}\big)$ of the new 0.95 confidence cube for $\theta = (\theta_{00}, \theta_{10}, \theta_{01}, \theta_{12})$. This cube was obtained using $c = 2$, $r = 8$ and $\lambda = 0.08$.

4. Illustration of the application of the new confidence cube

In this section we illustrate the application of the new $1 - \alpha$ confidence cube, utilizing the uncertain prior information, to a real data set. We extract a 2×2 factorial data set from the 2^3 factorial data set described in Table 7.5 of Box et al [20] as follows. Define $x_1 = -1$ and $x_1 = 1$ for "Time of addition of HNO_3" equal to 2 hours and 7 hours, respectively. Also define $x_2 = -1$ and $x_2 = 1$ for "heel absent" and "heel present", respectively. The observed responses are the following:

For $(x_1, x_2) = (-1, -1)$, $y = 87.2$.

For $(x_1, x_2) = (1, -1)$, $y = 88.4$.

For $(x_1, x_2) = (-1, 1)$, $y = 86.7$.

For $(x_1, x_2) = (1, 1)$, $y = 89.2$.

We use the model (1). The discussion on p.265 of Box et al [20] implies that there is uncertain prior information that $\beta_{12} = 0$. The discussion on p.266 of Box et al [20] implies that there is an estimator $\hat{\sigma}^2$ of σ^2, obtained from other related experiments, with the property that $\hat{\sigma}^2/\sigma^2 \sim Q/m$ where $Q \sim \chi^2_m$ and m is effectively infinite. The observed value of $\hat{\sigma}$ is 0.8. The standard 0.95 confidence cube for θ is

$$[87.2 \pm 1.99272] \times [88.4 \pm 1.99272] \times [86.7 \pm 1.99272] \times [89.2 \pm 1.99272].$$

We have also computed the new 0.95 confidence cube for θ, using $d = 6$, $\lambda = 0.08$ and equally-spaced knots at $0, 1, \ldots, 6$. This new confidence cube is

$$[87.1748 \pm 1.88504] \times [88.4252 \pm 1.88504] \times [86.7252 \pm 1.88504] \times [89.1748 \pm 1.88504].$$

Thus

$$\sqrt{\frac{(\text{volume of new 0.95 confidence cube})}{(\text{volume of standard 0.95 confidence cube})}} = 0.8948$$

For this data set, we have clearly gained by using the new 0.95 confidence cube for θ.

Remark The new $1 - \alpha$ confidence cube is computed to satisfy the constraint that its minimum coverage probability is $1 - \alpha$. For the examples described in both the previous section (for which $c = 2$, $r = 8$ and $\lambda = 0.08$) and the current section (for which c is effectively infinite, $r = 6$ and $\lambda = 0.08$), it is remarkable that the

new 0.95 confidence cube has coverage probability *equal* to 0.95 throughout the parameter space. The new 0.95 confidence cube was also computed for (a) $c = 3$, $r = 8$ and $\lambda = 0.08$, (b) $c = 7$, $r = 8$ and $\lambda = 0.08$ and (c) $c = 20$, $r = 8$ and $\lambda = 0.08$. In each of these cases, the new 0.95 confidence cube also has coverage probability *equal* to 0.95 throughout the parameter space. This provides strong empirical evidence that the new $1-\alpha$ confidence cube has the attractive property that its coverage probability is equal to $1-\alpha$ throughout the parameter space.

Appendix. Proof of Theorem 1

In this appendix we prove Theorem 1.

Proof of part (a).

Remember that $c(\gamma; b, s)$ is equal to (3). It follows from the $N(\gamma, 1)$ distribution of H and the independence of the random vectors (G_1, G_2, G_3, G_4, H) and W that (3) is equal to

$$\int_0^\infty \int_{-\infty}^\infty a(h,w)\,\phi(h-\gamma)\,dh\,f_W(w)\,dw,$$

where

$$\begin{aligned} a(h,w) =& P\big(\ell(h,w) \le G_1 \le u(h,w),\, \ell(h,w) \le -G_2 \le u(h,w), \\ & \qquad \ell(h,w) \le -G_3 \le u(h,w),\, \ell(h,w) \le G_4 \le u(h,w) \,\big|\, H = h\big). \end{aligned}$$

Recall the expressions for G_1, G_2, G_3 and G_4 in terms of T_1, T_2, T_3 and H. Also note that T_1, T_2, T_3 and H are independent random variables and that T_1, T_2 and T_3 are identically $N(0,1)$ distributed. Thus $T_1 - T_2$ and $T_1 + T_2$ are independent $N(0,2)$ distributed random variables and $a(h,w)$ is equal to

$$\begin{aligned} &\int_{-\infty}^\infty P\big(\ell_1 \le T_1 - T_2 \le u_1,\, -u_1 \le T_1 - T_2 \le -\ell_1, \\ &\qquad\qquad \ell_2 \le T_1 + T_2 \le u_2,\, -u_2 \le T_1 + T_2 \le -\ell_2\big)\,\phi(t_3)\,dt_3 \\ &= \int_{-\infty}^\infty P\big(\tilde{\ell}_1 \le T_1 - T_2 \le \tilde{u}_1\big) P\big(\tilde{\ell}_2 \le T_1 + T_2 \le \tilde{u}_2\big)\,\phi(t_3)\,dt_3 \\ &= \int_{-\infty}^\infty k(t_3, h, w, \gamma)\,\phi(t_3)\,dt_3 \end{aligned}$$

Thus $c(\gamma; b, s)$ is equal to

$$\int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty k(t_3, h, w, \gamma)\,\phi(t_3)\,dt_3\,\phi(h-\gamma)\,dh\,f_W(w)\,dw. \tag{A.1}$$

The standard $1-\alpha$ confidence cube I has coverage probability $1-\alpha$. Hence

$$1-\alpha = \int_0^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty k^\dagger(t_3, h, w, \gamma)\, \phi(t_3)\, dt_3\, \phi(h-\gamma)\, dh\, f_W(w)\, dw. \qquad \text{(A.2)}$$

Subtracting (A.2) from (A.1) and noting that, by Restriction 3, $b(x) = 0$ for all $|x| \geq r$ and $s(x) = d_{1-\alpha}$ for all $x \geq r$, we find that $c(\gamma; b, s)$ is equal to

$$(1-\alpha) + \int_0^\infty \int_{-rw}^{rw} \int_{-\infty}^\infty \big(k(t_3, h, w, \gamma) - k^\dagger(t_3, h, w\gamma)\big)\, \phi(t_3)\, dt_3\, \phi(h-\gamma)\, dh\, f_W(w)\, dw.$$

Changing the variable of integration from h to $x = h/w$, we obtain (6). It is straightforward to show that $P(\theta \in J(b,s))$ is an even function of γ.

Proof of part (b).

The random variables H and W are independent. Thus

$$e(\gamma; s) = \frac{1}{d_{1-\alpha}^4\, E(W^4)} \int_0^\infty \int_{-\infty}^\infty s^4\left(\frac{|h|}{w}\right) \phi(h-\gamma)\, dh\, w^4\, f_W(w)\, dw \qquad \text{(A.3)}$$

Obviously,

$$1 = \frac{1}{d_{1-\alpha}^4\, E(W^4)} \int_0^\infty \int_{-\infty}^\infty d_{1-\alpha}^4\, \phi(h-\gamma)\, dh\, w^4\, f_W(w)\, dw. \qquad \text{(A.4)}$$

Note that $s(x) = d_{1-\alpha}$ for all $x \geq r$. Subtracting (A.4) from (A.3), we therefore obtain

$$e(\gamma; s) = 1 + \frac{1}{d_{n-p,1-\alpha}^4\, E(W^4)} \int_0^\infty \int_{-rw}^{rw} \left(s^4\left(\frac{|h|}{w}\right) - d_{1-\alpha}^4\right) \phi(h-\gamma)\, dh\, w^4\, f_W(w)\, dw.$$

Changing the variable of integration from h to $x = h/w$, we obtain (7).

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